Persistent spin helix on a wurtzite ZnO(10 10) surface: First-principles density-functional study

著者	Absor Moh Adhib Ulil, Ishii Fumiyuki, Kotaka Hiroki, Saito Mineo
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Supplemental information for "Persistent spin helix on a wurtzite ZnO $(10\bar{1}0)$ surface: First-principles density-functional study"

Moh Adhib Ulil Absor[1,2], Fumiyuki Ishii[3], Hiroki Kotaka[1], and Mineo Saito[3]

[1]*Graduate School of Natural Science and Technology, Kanazawa University, Kanazawa 920-1192, Japan*
[2]*Department of Physics Universitas Gadjah Mada BLS 21 Yogyakarta Indonesia*
[3]*Faculty of Mathematics and Physics, Institute of Science and Engineering, Kanazawa University, Kanazawa 920-1192, Japan*

In this supplementary material, we present first-principles calculational results of the $[10\bar{1}0]$-oriented ZnO bulk system. Wurtzite ZnO forms a hexagonal close-packed lattice where the in-plane and axial lattice parameters are represented by a and c, respectively [Fig. 1 (a)]. The conventional unit vectors are given by $\vec{a}_1 = (1/2, \sqrt{3}/2, 0)a$, $\vec{a}_2 = (1/2, -\sqrt{3}/2, 0)a$, and $\vec{a}_3 = (0, 0, c/a)a$, where a and c are the lattice constants in the a and c-directions, respectively. The Zn atoms are located at $(0, 0, 0)$ and $(2/3, 1/3, 1/2)$ whereas the O atoms are located at $(0, 0, u)$ and $(2/3, 1/3, u + 1/2)$. The length of Zn-O bond along the c-axis is given by $d = uc$.

Here, we introduce new unit vectors which are suitable for describing non-polar $[10\bar{1}0]$ surfaces. The new unit vectors are $\vec{a}_1 = (1, 0, 0)a$, $\vec{a}_2 = (0, c/a, 0)a$, and $\vec{a}_3 = (0, 0, \sqrt{3})a$ with eight atoms per unit cell. In the new unit vectors, the polar [0001] and non-polar $[10\bar{1}0]$ directions are set to be the y and the z directions, respectively [Fig. 1 (b)]. Our calculations of the optimized lattice constants show that $a = 3.2845$ Å, $c = 5.3029$ Å, $c/a = 0.6151$, and $u = 0.3791$. These values are consistent with our previous results.[1)]

Here, we study the effect of SOC on the $[10\bar{1}0]$-oriented ZnO bulk system. We focus on the top of valence band maximum (VBM) along high symmetry line in the first Brillouin zone [Fig. 1(c)]. As shown in Fig. 2, the bands are spin degenerated in the Γ-Y direction, whereas they split in the Γ-X direction. In this spin-split band, the fully out-of-plane orientations of the spin textures are found [Fig. 3].

Considering the fact that this system has the in-plane electric field in the y directions, which originates from the polarity of the present system, the SOC can be expressed by $H_{SOC} = \alpha_1(k_x\sigma_z + k_z\sigma_x)$, where k_x and k_z are the wave vectors in the x and z directions, respectively σ_x and σ_z are the x and y components of Pauli matrixes. In this expression, α_1 is the Rashba spin-orbit strength, which is proporsional to the in-plane electric filed E_y. In the case that $k_z = 0$, only the first term of H_{SOC} remains. In this case, spin degenerated bands are induced in the Γ-Y direction and they split in the Γ-X direction [Fig. 2]. Furtheremore, due to the

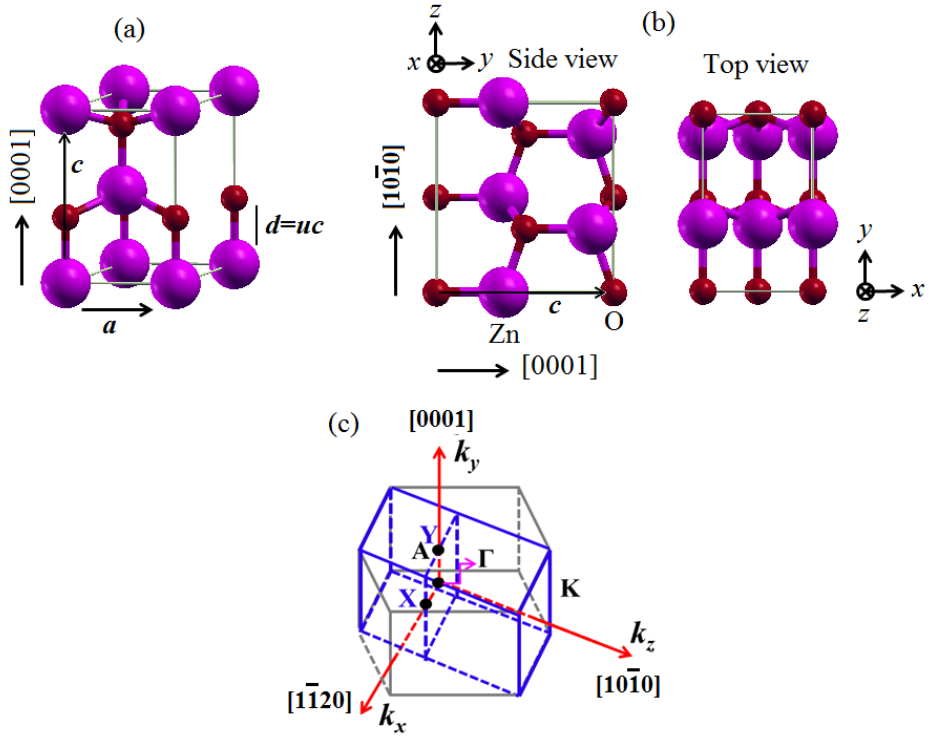

Fig. 1. Crystal structures of wurtzite bulk ZnO (a) and [10$\bar{1}$0]-oriented bulk ZnO (b) and first Brillouin zone (c). Black and blue lines represent the first Brillouin zone of the wurtzite bulk system and [10$\bar{1}$0]-oriented bulk system, respectively.

first term of H_{SOC}, the fully out-of-plane directions of the spin textures are generated [Fig. 3].

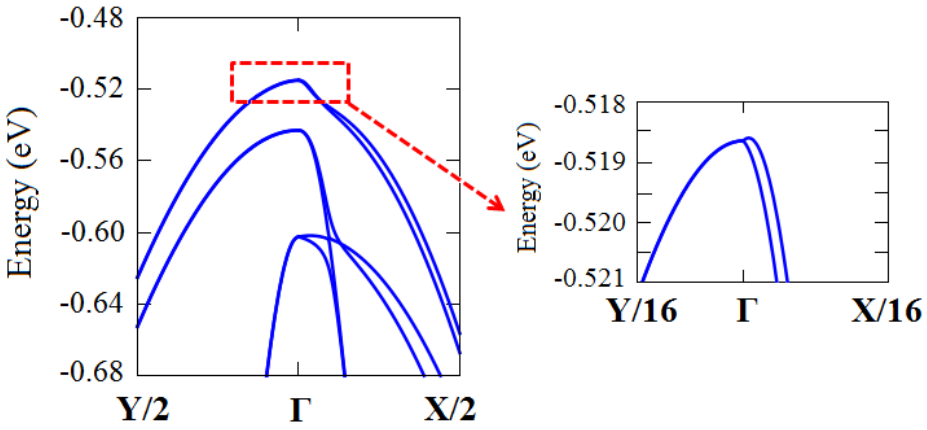

Fig. 2. Band structures near the VBM in the Y - Γ - X direction. The insert shows the spi-splitt band at the top of VBM.

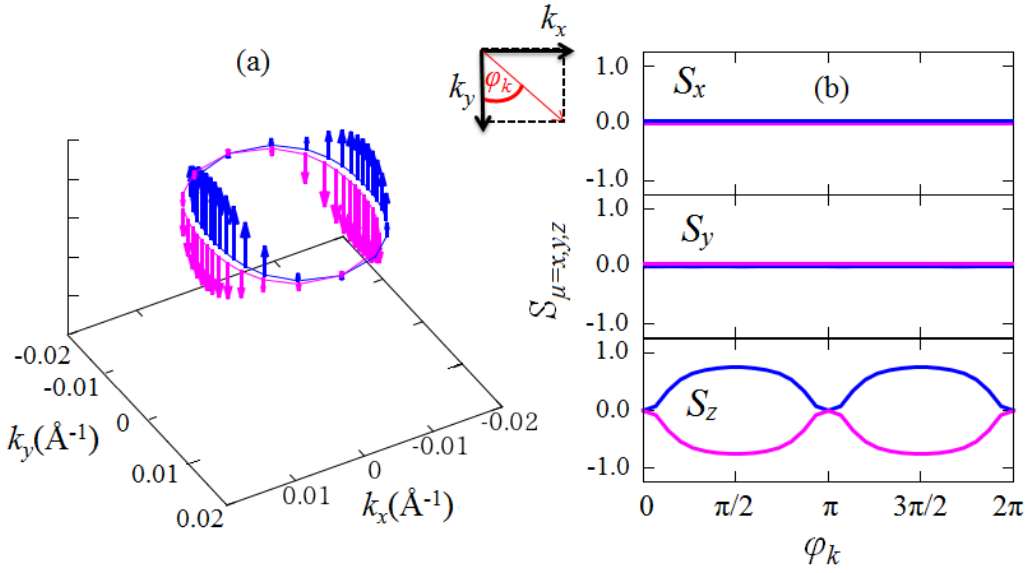

Fig. 3. (a) Spin textures of VBM. The band energy of the spin textures is 0.001 eV below the highest energy of the occupied states. The arrows represent the spin directions. The blue and pink lines correspond to iso-surfecae of the above-mentioned band energy. (b) Relationship between rotation angle (φ_k) and spin components.

References

1) M. A. U. Absor, H. Kotaka, F. Ishii, and M. Saito, Applied Physics Express 7, 053002 (2014).